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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2										
* * *	* *	* *	* *	* Welcome to STN International * * * * * * * * * *						
NEWS	1			Web Page for STN Seminar Schedule - N. America						
NEWS	2	AUG	06	CAS REGISTRY enhanced with new experimental property tags						
NEWS	3	AUG	06	FSTA enhanced with new thesaurus edition						
NEWS	4	AUG	13	CA/CAplus enhanced with additional kind codes for granted						
				patents						
NEWS	5	AUG	20	CA/CAplus enhanced with CAS indexing in pre-1907 records						
NEWS	6	AUG	27	Full-text patent databases enhanced with predefined						
				patent family display formats from INPADOCDB						
NEWS	7	AUG	27	USPATOLD now available on STN						
NEWS	8	AUG	28	CAS REGISTRY enhanced with additional experimental						
				spectral property data						
NEWS	9	SEP	07	STN AnaVist, Version 2.0, now available with Derwent						
				World Patents Index						
NEWS		SEP		FORIS renamed to SOFIS						
NEWS		SEP		INPADOCDB enhanced with monthly SDI frequency						
NEWS	12	SEP	17	CA/CAplus enhanced with printed CA page images from						
				1967-1998						
NEWS	13	SEP	17	CAplus coverage extended to include traditional medicine						
				patents						
NEWS		SEP		EMBASE, EMBAL, and LEMBASE reloaded with enhancements						
NEWS	15	OCT	02	CA/CAplus enhanced with pre-1907 records from Chemisches						
				Zentralblatt						
NEWS		OCT		BEILSTEIN updated with new compounds						
NEWS		NOV		Derwent Indian patent publication number format enhanced						
NEWS		NOV		WPIX enhanced with XML display format						
NEWS NEWS		NOV		ICSD reloaded with enhancements LINPADOCDB now available on STN						
		DEC								
NEWS NEWS		DEC		BEILSTEIN pricing structure to change USPATOLD added to additional database clusters						
NEWS NEWS		DEC	17	IMSDRUGCONF removed from database clusters and STN DGENE now includes more than 10 million sequences						
NEWS		DEC								
NEWS	25	DEC	1/	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment						
NEWS	26	DEC	17	MEDLINE segment MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary						
NEWS		DEC		CA/CAplus enhanced with new custom IPC display formats						
NEWS		DEC		STN Viewer enhanced with full-text patent content						
MEMO	20	DEC	1/	from USPATOLD						
NEWS	29	JAN	02	STN pricing information for 2008 now available						
NEWS	EXP	RESS		SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,						
				RRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0jc(JP),						
			ANI	D CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.						
NIELLO	HOTH	0.0	c.m	N Occasion Harris Bloom Bloom Ball Barris British						
NEWS				N Operating Hours Plus Help Desk Availability						
NEWS				lcome Banner and News Items						
NEWS	TPC	8	F.O1	r general information regarding STN implementation of IPC 8						

Enter NEWS followed by the item number or name to see news on that specific topic.

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=> ile registry

ILE IS NOT A RECOGNIZED COMMAND

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=> file registry

COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE ENTRY

NTRY SESSION 0.21 0.21

TOTAL

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STRUCTURE FILE UPDATES: 7 JAN 2008 HIGHEST RN 960112-28-1 DICTIONARY FILE UPDATES: 7 JAN 2008 HIGHEST RN 960112-28-1

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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http://www.cas.org/support/stngen/stndoc/properties.html

= \

Uploading C:\Program Files\STNEXP\Queries\10581255e.str

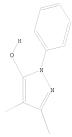


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12 13 14 15
ring nodes:
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chain bonds:
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ring bonds:
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11
exact/norm bonds:
1-2 1-5 2-3 3-4 4-5 4-13 5-6
exact bonds:
2-12 3-15 13-14
normalized bonds:
6-7 6-11 7-8 8-9 9-10 10-11

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS

L1 STRUCTURE UPLOADED

=> D L1 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L1 fam full

FULL SEARCH INITIATED 15:43:52 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 4156 TO ITERATE

100.0% PROCESSED 4156 ITERATIONS SEARCH TIME: 00.00.01

1 ANSWERS

L2 1 SEA FAM FUL L1

=> D L2

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN RN $370557{-}61{-}2$ REGISTRY

ED Entered STN: 17 Nov 2001

CN 1H-Pyrazol-5-ol, 3,4-dimethyl-1-phenyl- (CA INDEX NAME)

MF C11 H12 N2 O SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE) => file caplus COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 72 57 72.78

FILE 'CAPLUS' ENTERED AT 15:44:08 ON 08 JAN 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 8 Jan 2008 VOL 148 ISS 2 FILE LAST UPDATED: 7 Jan 2008 (20080107/ED)

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=> s L2

SOURCE:

1 L2 L3

=> D L3 ibib abs kwic

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:591008 CAPLUS

DOCUMENT NUMBER: 135:331163

TITLE: Tautomerism in 4-substituted 1-phenyl-3-methyl-

pyrazolin-5-ones-a theoretical ab initio and 13C NMR

study

AUTHOR(S): Kleinpeter, E.; Koch, A.

CORPORATE SOURCE: Institut fur Organische Chemie und Strukturanalytik.

Universitat Potsdam, Potsdam, D-14415, Germany Journal of Physical Organic Chemistry (2001), 14(8),

566-576

CODEN: JPOCEE; ISSN: 0894-3230

John Wiley & Sons Ltd. PUBLISHER:

DOCUMENT TYPE: Journal

LANGUAGE:

English The tautomeric equilibrium between the CH, OH and NH forms in a series of 4-substituted 1-phenyl-3-methyl-pyrazolin-5-ones have been studied using ab initio calcus, at various levels of theory and comparison made with the exptl. results obtained from NMR measurements. Quant. comparison of both the relative energies and the 13C chemical shifts of the tautomers constituting the tautomeric equilibrium were made by calcn. of both sets of parameters. The influence of the solvent was included by employing various models of the self-consistent reaction field theory. Initially, the solvent was included in the calcns. by applying a continuum of differing polarity over the surface of isolated tautomers (self-consistent isodensity polarized continuum model method), then later by assuming formation of an adduct between the solute and the solvent (thereby

simulating effectively the hydrogen bonding in the OH and NH tautomers) and finally by calculating dimer or trimer complexes of the various tautomers. In this manner, the agreement between the theor. calculated and the exptl. determined tautomeric equilibrium was improved significantly. The theor. calculated 13C

chemical shifts of the tautomers were found to be viable for the assignment of the tautomers, particularly the preferred tautomer in the OH/NH equilibrium, which remains fast on the NMR time scale even at low temps.

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

89-25-8, 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-2-phenyl-1H-Pvrazol-5-ol, 3-methyl-1-phenyl- 2721-84-8 4173-74-4, 3H-Pyrazol-3-one, 4-acetyl-2, 4-dihydro-5-methyl-2-phenyl- 6077-03-8 7713-77-1, 3H-Pyrazol-3-one, 1,2-dihydro-4,5-dimethyl-2-phenyl-17900-68-4, 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl-19735-89-8, 3H-Pyrazol-3-one, 1,2-dihydro-5-methyl-2-phenyl- 27852-31-9 37703-59-6 40864-30-0, 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-4-nitro-2phenyl- 41927-23-5, 3H-Pyrazol-3-one, 4-bromo-2, 4-dihydro-5-methyl-2phenyl- 52944-72-6 56634-79-8 64598-47-6 68719-56-2, 3H-Pyrazol-3-one, 4-bromo-1,2-dihydro-5-methyl-2-phenyl-1H-Pyrazol-5-ol, 4-bromo-3-methyl-1-phenyl- 78575-99-2, 1H-Pvrazol-5-ol,3-methvl-4-nitro-1-phenvl- 78576-03-1 138740-34-8 370557-61-2 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(ab initio and 13C NMR study of tautomerism in 4-substituted 1-phenyl-3-methyl-pyrazolin-5-ones)

=> file registry COST IN U.S. DOLLARS SINCE FILE TOTAL SESSION ENTRY FULL ESTIMATED COST 6.15 78.93 DISCOUNT AMOUNTS (FOR OUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -0.80 -0.80

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

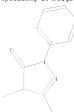
Please note that search-term pricing does apply when conducting ${\tt SmartSELECT}$ searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\STNEXP\Queries\10581255f.str



chain nodes : 12 13 14

ring nodes:
1 2 3 4 5 6 7 8 9 10 11
chain bonds:
2-12 3-14 4-13 5-6
ring bonds:
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11
exact/norm bonds:
1-2 1-5 2-3 3-4 4-13 4-5 5-6
exact bonds:
2-12 3-14
normalized bonds:
6-7 6-11 7-8 8-9 9-10 10-11

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS

L4 STRUCTURE UPLOADED

=> D L4 L4 HAS NO ANSWERS L4 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s L4 fam full
FULL SEARCH INITIATED 15:48:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -
                                  4156 TO ITERATE
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100.0% PROCESSED 4156 ITERATIONS SEARCH TIME: 00.00.01

L5 2 SEA FAM FUL L4

=> D L5

- L5 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2008 ACS on STN RN 152968-73-5 REGISTRY
- ED
- Entered STN: 11 Feb 1994
- CN Pentanoic acid, 5-amino-4-oxo-, mixt. with 2,4-dihydro-4,5-dimethyl-2phenyl-3H-pyrazol-3-one (9CI) (CA INDEX NAME) OTHER CA INDEX NAMES:

2 ANSWERS

- CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl-, mixt. contg. (9CI)
- MF C11 H12 N2 O . C5 H9 N O3
- CI MXS SR CA
- STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 17900-68-4

CMF C11 H12 N2 O

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CM 2
    CRN 106-60-5
    CMF C5 H9 N O3
H2N-CH2-C-CH2-CH2-CO2H
              1 REFERENCES IN FILE CA (1907 TO DATE)
              1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
=> 1-2
1-2 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).
=> D L5 1-2
    ANSWER 1 OF 2 REGISTRY COPYRIGHT 2008 ACS on STN
     152968-73-5 REGISTRY
    Entered STN: 11 Feb 1994
    Pentanoic acid, 5-amino-4-oxo-, mixt. with 2,4-dihydro-4,5-dimethyl-2-
    phenyl-3H-pyrazol-3-one (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl-, mixt. contq. (9CI)
    C11 H12 N2 O . C5 H9 N O3
    MXS
    CA
    STN Files: CA, CAPLUS, USPATFULL
    CM 1
     CRN 17900-68-4
     CMF C11 H12 N2 O
     CM
    CRN 106-60-5
    CMF C5 H9 N O3
H2N-CH2-C-CH2-CH2-CO2H
```

ED

MF

CI

SR

LĊ

- 1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 17900-68-4 REGISTRY
- ED Entered STN: 16 Nov 1984
- CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
- CN 2-Pyrazolin-5-one, 3,4-dimethyl-1-phenyl- (6CI, 7CI, 8CI) OTHER NAMES:
- CN 1-Phenyl-3, 4-dimethylpyrazolin-5-one
- CN 3,4-Dimethyl-1-phenyl-2-pyrazolin-5-one
- CN 3,4-Dimethyl-1-phenylpyrazolone
- MF C11 H12 N2 O
- CI COM
- LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, IFICDB, IFIPAT, IFIUDB, MSDS-OHS, TOXCENTER, USPATFULL, USPATOLD ("File contains numerically searchable property data)
 - Other Sources: EINECS**

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- 38 REFERENCES IN FILE CA (1907 TO DATE)
- 38 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
- => file caplus SINCE FILE COST IN U.S. DOLLARS TOTAL. ENTRY SESSION FULL ESTIMATED COST 76.57 155.50 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -0.800.00

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=> d his

(FILE 'HOME' ENTERED AT 15:42:32 ON 08 JAN 2008)

FILE 'REGISTRY' ENTERED AT 15:42:46 ON 08 JAN 2008

L1 STRUCTURE UPLOADED

L2 1 S L1 FAM FULL

FILE 'CAPLUS' ENTERED AT 15:44:08 ON 08 JAN 2008 L3 1 S L2

FILE 'REGISTRY' ENTERED AT 15:47:41 ON 08 JAN 2008

L4 STRUCTURE UPLOADED L5 2 S L4 FAM FULL

FILE 'CAPLUS' ENTERED AT 15:49:00 ON 08 JAN 2008

=> s L5 L6 39 L5

=> S L6 and (py<2003 or ay <2003 or pry<2003)

22927520 PY<2003 4474522 AY <2003

3949553 PRY<2003 .7 36 L6 AND (PY<2003 OR AY <2003 OR PRY<2003)

=> D L7 1-10 ibib abs kwic hitstr

L7 ANSWER 1 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:921440 CAPLUS

DOCUMENT NUMBER: 139:391385

TITLE: Pyrazolone analogs for repairing tissue fibrosis
INVENTOR(S): Chiba, Akira; Matsumoto, Hideki; Tanaka, Yasuhiro;
Ijichi, Chiori; Oomuta, Naoko; Takatsuki, Fumihiko

PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent
LANGUAGE: Japanese

LANGUAGE: Jag FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003335672	A	20031125	JP 2002-144720	20020520 <
PRIORITY APPLN. INFO.:			JP 2002-144720	20020520 <
OTHER SOURCE(S):	MARPAT	139:391385		

Pyrazolone analogs (I; R1 = (substituted)phenyl; R2, R3 = H; R4 = low alkyl, alkoxy, etc.) and their pharmaceutically acceptable salts are claimed for repairing tissue fibrosis, including liver fibrosis, lung fibrosis, kidney fibrosis, atherosclerosis, prostate hypertrophy, keloid symptom, myocardial symptom, and collagen disease.

PATENT NO. KIND DATE APPLICATION NO. ----------20031125 JP 2002-144720 20020520 <--JP 2003335672 20020520 <--PRAI JP 2002-144720 90-31-3 4845-49-2 6402-09-1 6631-89-6 13024-90-3 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pyrazolone analogs for repairing tissue fibrosis) 17900-68-4 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pyrazolone analogs for repairing tissue fibrosis)

3H-Pyrazo1-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)

RN

CN

L7 ANSWER 2 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:757683 CAPLUS

DOCUMENT NUMBER: 139:261293

TITLE: Preventive and/or therapeutic agent for hypoxic

ischemic brain disorder

Ikeda, Tomoaki; Ikenoue, Tsuyomu INVENTOR(S): Mitsubishi Pharma Corporation, Japan PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 29 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

17900-68-4 CAPLUS

PATENT INFORMATION:

PAT	ENT	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		Di	ATE	
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                                                                  20030314 <--
PRIORITY APPLN. INFO .:
                                           JP 2002-71595
                                                               A 20020315 <--
                                           WO 2003-JP3067
                                                               W 20030314
OTHER SOURCE(S):
                        MARPAT 139:261293
    The patent relates to a medicine for use in the prevention of and/or
AB
    treatments for hypoxic ischemic brain disorders, especially ones of newborns
    caused by labor. It contains as an active ingredient a substance selected
    from the group consisting of 3-methyl-1-phenyl-2-pyrazolin-5-one,
    pyralozone derivs. which are analogs thereof, physiol. acceptable salts
    thereof, and any hydrates and any solvates of these. Thus,
    1-phenyl-3-methyl-2-pyrazolin-5-one prepared by refluxing Et acetoacetate
    with phenylhydrazine in ethanol and recrystn, was dissolved in simulated
    body fluid and showed effect on hypoxic ischemic brain of new born rat.
    PATENT NO.
                        KIND
                               DATE
                                          APPLICATION NO.
                                         WO 2003-JP3067
    WO 2003078401
                         A1
                               20030925
                                                                 20030314 <--
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            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
            LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH,
            PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
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                 60798-13-2 60875-16-3 65156-70-9 70972-70-2
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                 602297-82-5 602297-84-7 602297-85-8 602297-86-9
    602297-64-3
    602297-87-0
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (pyrazolinone derivative for preventive and/or therapeutic agent for
       hypoxic ischemic brain disorder)
IT
    17900-68-4
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (pyrazolinone derivative for preventive and/or therapeutic agent for
       hypoxic ischemic brain disorder)
RN
    17900-68-4 CAPLUS
    3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)
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ΡI



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:591008 CAPLUS

DOCUMENT NUMBER: 135:331163

TITLE: Tautomerism in 4-substituted 1-phenyl-3-methyl-

pyrazolin-5-ones-a theoretical ab initio and 13C NMR

study

AUTHOR(S): Kleinpeter, E.; Koch, A.

CORPORATE SOURCE: Institut fur Organische Chemie und Strukturanalytik, Universitat Potsdam, Potsdam, D-14415, Germany

SOURCE: Journal of Physical Organic Chemistry (2001

), 14(8), 566-576

CODEN: JPOCEE; ISSN: 0894-3230 PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

The tautomeric equilibrium between the CH, OH and NH forms in a series of 4-substituted 1-phenyl-3-methyl-pyrazolin-5-ones have been studied using ab initio calcns. at various levels of theory and comparison made with the exptl. results obtained from NMR measurements. Quant. comparison of both the relative energies and the 13C chemical shifts of the tautomers constituting the tautomeric equilibrium were made by calcn. of both sets of parameters. The influence of the solvent was included by employing various models of the self-consistent reaction field theory. Initially, the solvent was included in the calcns. by applying a continuum of differing polarity over the surface of isolated tautomers (self-consistent isodensity polarized continuum model method), then later by assuming formation of an adduct between the solute and the solvent (thereby simulating effectively the hydrogen bonding in the OH and NH tautomers) and finally by calculating dimer or trimer complexes of the various tautomers. In this manner, the agreement between the theor, calculated and the exptl. determined tautomeric equilibrium was improved significantly. The theor. calculated 13C

chemical shifts of the tautomers were found to be viable for the assignment of the tautomers, particularly the preferred tautomer in the OH/NH equilibrium, which remains fast on the NMR time scale even at low temps.

SO Journal of Physical Organic Chemistry (2001), 14(8), 566-576 CODEN: JPOCEE; ISSN: 0894-3230

IT 89-25-8, 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-2-phenyl- 942-32-5, 1H-Pyrazol-5-ol,3-methyl-1-phenyl- 2721-84-8 4173-74-4, 3H-Pyrazol-3-one, 4-acetyl-2,4-dihydro-5-methyl-2-phenyl- 6077-03-8 7713-77-1, 3H-Pyrazol-3-one, 1,2-dihydro-4,5-dimethyl-2-phenyl- 17900-68-4, 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-2-phenyl- 19735-89-8, 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-2-phenyl- 27852-31-9 37703-59-6 40864-30-0, 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-4-nitro-2-phenyl- 41927-23-5, 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-2-phenyl- 52944-72-6 56634-79-8 64598-47-6 68719-56-2, 3H-Pyrazol-3-one, 4-bromo-1,2-dihydro-5-methyl-2-phenyl- 78575-98-1, 1H-Pyrazol-3-one, 4-bromo-3-methyl-1-phenyl- 78575-99-2, 1H-Pyrazol-5-ol,4-bromo-3-methyl-1-phenyl- 78575-99-2, 1H-Pyrazol-5-ol,3-methyl-4-nitro-1-phenyl- 78576-03-1 138740-34-8

370557-61-2

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(ab initio and 13C NMR study of tautomerism in 4-substituted 1-pheny1-3-methy1-pyrazolin-5-ones)

IT 17900-68-4, 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenylRL: PEP (Physical, engineering or chemical process); PRP (Properties);
PROC (Process)

(ab initio and 13C NMR study of tautomerism in 4-substituted 1-phenyl-3-methyl-pyrazolin-5-ones)

RN 17900-68-4 CAPLUS

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:361602 CAPLUS DOCUMENT NUMBER: 135:152747

DOCUMENT NUMBER: 135:152747
TITLE: Solid-phase synthesis of substituted pyrazolones from

polymer-bound β-keto esters
AUTHOR(S): Tietze, Lutz F.; Evers, Holger; Hippe, Thomas;

Steinmetz, Adrian; Topken, Enno

CORPORATE SOURCE: Institut fur Organische Chemie der

Georg-August-Universitat Gottingen, Gottingen, 37077,

Germany

SOURCE: European Journal of Organic Chemistry (2001

), (9), 1631-1634 CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Wiley-vch verlag Gmbh

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:152747

B. Polymer-bound acetoacetate was y-mono- and y-dialkylated, as well as a-monoalkylated. Treatment with hydrazine or substituted hydrazines followed by thermal or acidic cyclizing cleavage yielded the pyrazolones in a purity of >90%.

SO European Journal of Organic Chemistry (2001), (9), 1631-1634

CODEN: EJOCFK; ISSN: 1434-193X

IT 6402-09-1P 7058-21-1P 13051-47-3P 17900-68-4P 22717-41-5P 24246-68-0P 24246-11-5P 26502-95-4P 26618-09-0P 28844-37-3P 40339-61-5P 55294-29-6P 64123-72-4P 76552-51-7P 90688-89-4P 94575-26-5P 118031-38-2P 118049-09-5P 181185-05-7P B1185-07-9P 181185-09-1P 192209-24-6P 192209-25-9P 192209-26-0P 192209-27-1P 192209-28-2P 352434-76-5P 352434-77-6P RL: SPN (Synthetic preparation); FREP (Preparation)

(solid-phase synthesis of substituted pyrazolones from polymer-bound

β-keto esters)

IT 17900-68-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (solid-phase synthesis of substituted pyrazolones from polymer-bound B-keto esters)

RN 17900-68-4 CAPLUS

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1997:390186 CAPLUS

DOCUMENT NUMBER: 127 - 95230

TITLE: Solid-phase synthesis of polymer-bound B-keto esters and their application in the synthesis of

structurally diverse pyrazolones AUTHOR(S): Tietze, Lutz F.; Steinmetz, Adrian; Balkenhohl,

Friedhelm Inst. Org. Chem., Georg-August-Univ. Gottingen, CORPORATE SOURCE:

Gottingen, D-37077, Germany Bioorganic & Medicinal Chemistry Letters (1997 SOURCE:

), 7(10), 1303-1306

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier DOCUMENT TYPE: Journal LANGUAGE: English

Polymer-bound esters of HO2CCHR2COR1 [R1 = CH2Ph, CH2CH2CO2Me, (CH2)3Cl, cyclohexyl, Me; R2 = Me, Et, allyl, CH2CH:CMe2, hexyl,CH2CO2Et] were prepared by treating R1COCl with Meldrum's acid, treating the adduct with polymer-bound ethylene glycol, and alkylating the polymer-bound esters. Mild acid catalyzed reaction with phenylhydrazine or hydrazine occurred with cleavage from the resin and cyclization to give pyrazolones in high purity and good yield.

SO Bioorganic & Medicinal Chemistry Letters (1997), 7(10), 1303-1306

CODEN: BMCLE8; ISSN: 0960-894X

24246-11-5P 17900-68-4P 22717-41-5P 24246-08-0P 26502-95-4P 26645-09-0P 28844-37-3P 90688-89-4P 192209-24-8P 192209-25-9P 192209-26-0P 192209-27-1P 192209-28-2P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of polymer-bound β -keto esters and their conversion to pyrazolones)

17900-68-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of polymer-bound β -keto esters and their conversion to pyrazolones)

17900-68-4 CAPLUS

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)

RN

L7 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:659311 CAPLUS

DOCUMENT NUMBER: 125:300995

TITLE: Preparation of 2-pyrazoline derivatives as herbicides INVENTOR(S): Araino, Nobuyuki; Miura, Juzo; Oda, Yoshiki; Nishioka,

Hitoshi

PATENT ASSIGNEE(S): Nihon Nohyaku Co Ltd, Japan SOURCE: Jpn. Kokai Tokkyo Koho, 63 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08217777 PRIORITY APPLN. INFO.:	A	19960827	JP 1995-46427 JP 1995-46427	19950210 < 19950210 <
OTHER SOURCE(S): GI	MARPAT	125:300995		

AB The title compds. [I; R = (un)substituted alkyl or alkenyl or Ph or pyridinyl, etc.; Rl, R2 = H, (un)substituted alkyl or alkenyl, etc.; X = halo, NO2, (un)substituted alkyl or amino, etc.; n = 0-5; Z = CH2O] and their intermediates (Z = 0, :CH2; others are same as above) are claimed. Herbicides containing I are effective against Amaranthus lividus, Scirpus juncoides, and Monochoria vaginalis. Thus, trimethylsulfonium iodide was treated with NaH and then reacted with 4-benzoylmethyl-4-ethyl-3-methyl-1-phenyl-2-pyrazolin-5-one to give 55% a mixture of diastereoisomers I (R = Ph, R1 = Et, R2 = Me, X = H, n = 5, Z = CH2O) (II). Herbicides containing II at 3 kg/ha preemergence showed 100% herbicidal effect for Amaranthus lividus and Scirpus juncoides.

PI JP 08217777 A 19960827 Heisei

PA	TENT NO.	KIND	DATE	APPLICATION NO.	DATE		
	08217777 1995-46427	A	19960827 19950210 <	JP 1995-46427 	19950210 <		

II 106-95-6, Allyl bromide, reactions 2181-42-2, Trimethylsulfonium iodide 7534-40-9 17900-68-4 41011-01-2, 3-Chlorophenacyl bromide 182875-62-3

RL: RCT (Reactant); RACT (Reactant or reagent)

Ι

(preparation of pyrazoline derivs. as herbicides)

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of pyrazoline derivs. as herbicides)
RN 17900-68-4 CAPLUS

CN 3H-Pyrazo1-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)



L7 ANSWER 7 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN 1995:133733 CAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER: 123:142959

TITLE: Steering effects of phase transfer catalysts on the benzylation of 2-naphtholate and the methylation of

3-methyl-1-phenyl-5-pyrazolone

Dehmlow, Eckehard V.; Klauck, Robert AUTHOR(S):

CORPORATE SOURCE: Fakultat Chemie, Univ. Bielefeld, Bielefeld, D-33615,

Germany SOURCE:

Journal of Chemical Research, Synopses (1994), (11), 448-9

CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:142959

O- vs. C-alkylation and bis-alkylation of 2-naphthol and O-, N- and C-alkylation or bis-alkylation of 3-methyl-1-phenyl-5-pyrazolone can be influenced by the nature and the presence of the phase transfer (PT) catalyst.

SO Journal of Chemical Research, Synopses (1994), (11), 448-9 CODEN: JRPSDC; ISSN: 0308-2342

17900-68-4

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)

(chemoselectivity by phase transfer catalysts in methylation of 3-methyl-1-phenyl-5-pyrazolone)

17900-68-4

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (chemoselectivity by phase transfer catalysts in methylation of

3-methyl-1-phenyl-5-pyrazolone)

17900-68-4 CAPLUS RN

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)



L7 ANSWER 8 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:127807 CAPLUS

DOCUMENT NUMBER: 120:127807

TITLE: Herbicidal δ -aminolevulinic acid combinations with chlorophyll biosynthesis modulators.

INVENTOR(S): Rebeiz, Constantin A. PATENT ASSIGNEE(S): SOURCE: Board of Trustees of the University of Illinois, USA U.S., 40 pp. Cont.-in-part of U.S. 5,163,990. CODEN: USXXAM Patent

DOCUMENT TYPE: LANGUAGE:

LANGUAGE: English FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PA	TENT NO.			KIN	D	DATE	AP	PLICATION NO.		DATE	
US	5242892			A	-	19930907	US	1990-615413 1989-106579		19901119	<
EP	331211			A2		19890906	EP	1989-106579		19850717	<
EP	331211			A3		19891123					
						GB, IT,	LI, L	U, NL, SE			
ZA	8505561 5127938			A		19860326	ZA	1985-5561		19850723	<
US	5127938			A		19920707	US	1986-895529		19860811	<
US	5200427			A				1989-294132			
	5163990			A				1990-521119			
								1991-2080140		19910502	<
	2080140			C		20020108					
WO						19911114	WO	1991-US3015		19910502	<
	W: CA,										
		BE,	CH,					R, IT, LU, NL			
EP	527186			A1		19930217	EP	1991-909022		19910502	<
	R: BE,	CH,	DE,	DK,	ES.	, FR, GB,	GR, I	T, LI, NL 1991-508902 1991-2358003 1991-773030 1991-795367 1992-915896 2000-226123			
JP	06500989 2358003 5286708 5300526 5321001 20011516 3365503			T		19940127	JP	1991-508902		19910502	<
CA	2358003			С		20020924	CA	1991-2358003		19910502	<
US	5286708			A		19940215	US	1991-773030		19911008	<
US	5300526			A		19940405	US	1991-795367		19911120	<
US	5321001			A		19940614	US	1992-915896		19920717	<
JP	20011516	14		A		20010605	JP	2000-226123		20000621	<
JP	3365503			B2		20030114					
JP	20030639	0.7		A			JP	2002-236923		20020815	<
JP	3734780 Y APPLN.			B2		20060111					
PRIORIT	Y APPLN.	INFO	. :					1984-634932			
								1985-754092		19850715	
								1986-895529		2 19860811	
								1990-521119		2 19900503	
								1985-903637			
								1988-144883			
								1989-294132		3 19890109	
								1990-615413		19901119	
							CA	1991-2080140	A.	3 19910502	
							JP	1991-508902	A.	3 19910502	
							WO	1991-US3015	W	19910502	<
							JP	2000-226123	A.	3 20000621	<

AB The title compns. are defoliants and herbicides, with activity based on the accumulation of photodynamic tetrapyrrols. A mixture of 20 mM γ -aminolevulinic acid and 15 mM 6-aminonicotinic acid defoliated tomato seedlings.

PI	US	5242	892	A	19930	0907								
	PA:	TENT :	NO.			KINI)	DATE	3	API	PLICAT	ION NO.	DATE	
							-						 	
PI	US	5242	892			A		1993	0907	US	1990-	615413	19901119	<
	EP	3312	11			A2		1989	0906	EP	1989-	106579	19850717	<
	EP	3312	11			A3		1989	1123					
		R:	AT,	BE,	CH,	DE,	FR,	GB,	IT,	LI, LU	J, NL,	SE		
	ZA	8505	561			A		1986	0326	ZA	1985-	5561	19850723	<
	US	5127	938			A		1992	20707	US	1986-	895529	19860811	<
	US	5200	427			A		1993	0406			294132	19890109	<
	US	5163	990			A		1992	21117	US	1990-	521119	19900503	<
	CA	2080	140			A1		1991	1104	CA	1991-	2080140	19910502	<

	CA 2080140	C	20020108		
	WO 9116820	A1	19911114	WO 1991-US3015	19910502 <
		JP, KR			
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	EP 527186	A1	19930217	EP 1991-909022	19910502 <
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	JP 06500989	Т	19940127	JP 1991-508902	19910502 <
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	US 5300526	A	19940405	US 1991-795367	19911120 <
	US 5321001	A	19940614	US 1992-915896	19920717 <
	JP 200115161		20010605	JP 2000-226123	20000621 <
	JP 3365503	B2	20030114		
	JP 200306390	7 A	20030305	JP 2002-236923	20020815 <
	JP 3734780	B2	20060111		
PRAI	US 1984-6349	32 B2	19840727 <-	-	
	US 1985-7540	92 B1	19850715 <-	_	
	US 1986-8955		19860811 <-		
	US 1990-5211		19900503 <-		
	EP 1985-9036		19850717 <-		
	US 1988-1448		19880113 <-		
	US 1989-2941		19890109 <-		
	US 1990-6154		19901119 <-		
	CA 1991-2080		19910502 <-	-	
	JP 1991-5089	02 A3	19910502 <-	-	
	WO 1991-US30	15 W	19910502 <-	_	
	JP 2000-2261	23 A3	20000621 <-	-	
IT	117060-73-8	126840-94-6	126840-95-7	126841-05-2	126841-06-3
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	152969-01-2	152969-02-3	153145-67-6	i	
		icultural use); BAC (Biolog	ical activity or	effector, except
					iological study);
	HSES (Heas)	. ,		,,	, , , ,

USES (Uses)

(herbicide and defoliant)

152968-73-5

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(herbicide and defoliant)

152968-73-5 CAPLUS RN

CN Pentanoic acid, 5-amino-4-oxo-, mixt. with 2,4-dihydro-4,5-dimethyl-2phenyl-3H-pyrazol-3-one (9CI) (CA INDEX NAME)

CM 1

CRN 17900-68-4 CMF C11 H12 N2 O

CM

CRN 106-60-5 CMF C5 H9 N O3

L7 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:223017 CAPLUS

DOCUMENT NUMBER: 118:223017

TITLE: Nonsubstantive color developer for color filter and its use in manufacturing color filter for color

liquid crystal display INVENTOR(S):

Shimizu, Hiroshi; Miyaoka, Kazuyoshi; Hirota, Kenji; Koboshi, Shigeharu

PATENT ASSIGNEE(S):

Konica Co., Japan Jpn. Kokai Tokkyo Koho, 16 pp. SOURCE: CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04009053	A	19920113	JP 1990-109583	19900425 <
PRIORITY APPLN. INFO.:			JP 1990-109583	19900425 <



A nonsubstantive color developer for a color filter contains a high concentration

of Br- ion and ≥1 bias coupler [I; R = (un)substituted alkyl or aryl substituted at the active site; X = atoms required to form an (un)substituted (ring-fused) 5- or 6-membered ring containing ≥1 N, S, or O; the heterocyclic ring or the alkyl group is substituted with a C2-24 organic group which allows I to completely or partially dissolve in a processing solution and after coupling with the oxidized color developing agent, imparts I a mol. size and shape nondiffusible in an emulsion layer]. The Br- concentration is preferably ≥0.05 mol/L. A color filter is manufactured by (1) pattern-wise exposure of a photosensitive material having a Ag halide emulsion layer containing Ag halide micrograins formed on a transparent substrate and (2) nonsubstantive development by the above nonsubstantive color developer to form dve images corresponding to the patterns. The process reduces relief between pixels with different spectral characteristics, thus gives excellent surface smoothness, prevents fog in the unexposed parts, and gives sufficient d. in the exposed parts.

19920113 KIND	Heisei DATE	APPLICATION NO.	DATE
A			19900425 <
	19900425	<	
25740-63-8	131443-12	-4 147163-78-8	
	KIND A	A 19920113 19900425	KIND DATE APPLICATION NO.

RL: USES (Uses)

(bias coupler, nonsubstantive color developer containing bromide ions and, for color filter) 17900-68-4

RL: USES (Uses)

(bias coupler, nonsubstantive color developer containing bromide ions and, for color filter)

RN 17900-68-4 CAPLUS

3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME) CN

L7 ANSWER 10 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:52993 CAPLUS

DOCUMENT NUMBER: 114:52993

TITLE: Color filter for liquid-crystal color display device INVENTOR(S): Mochizuki, Yoshiharu; Okauchi, Ken; Masukawa, Toyoaki

PATENT ASSIGNEE(S): Konica Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.

CODEN: JKXXAF DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 02191903 A 19900727 JP 1989-79302 19890329 <-PRIORITY APPLN. INFO.: JP 1988-241800 A1 19880927 <--

AP A process for making a color filter for a liquid-crystal color display device comprises forming color images from a patternwise exposed Ag halide emulsion layer on a transparent support, using a developer solution containing couplers and color developing agents, wherein the images are treated with a processing solution containing a coupler capable of forming a substantially color-less compound by reacting with the oxidized color developing agent and

having a pH ≥9 at 25°.

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	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PT	JP 02191903	A	19900727	JP 1989-79302	19890329 <
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PRAI	JP 1988-241800	A1	19880927 <-	-	
IT	17900-68-4 72	705-83-0	119105-62-3	131443-12-4 13144	13-13-5
	131443-14-6 1:	31443-15-7	131443-16-8	131443-17-9 131	1443-18-0

RL: USES (Uses)
(obotog. processing solns, containing, for fabrication of color filters for

liquid-crystal display devices)
IT 17900-68-4

RL: USES (Uses)

(photog. processing solns. containing, for fabrication of color filters for liquid-crystal display devices)

RN 17900-68-4 CAPLUS

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)

=> D his

(FILE 'HOME' ENTERED AT 15:42:32 ON 08 JAN 2008)

FILE 'REGISTRY' ENTERED AT 15:42:46 ON 08 JAN 2008 L1 STRUCTURE UPLOADED

L2 1 S L1 FAM FULL

FILE 'CAPLUS' ENTERED AT 15:44:08 ON 08 JAN 2008 L3 1 S L2

FILE 'REGISTRY' ENTERED AT 15:47:41 ON 08 JAN 2008 L4 STRUCTURE UPLOADED

L5 2 S L4 FAM FULL

FILE 'CAPLUS' ENTERED AT 15:49:00 ON 08 JAN 2008

L6 39 S L5 L7 36 S L6 AND (PY<2003 OR AY <2003 OR PRY<2003) => logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y) /N/HOLD: y COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

71.66

227.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE

-8.00

-8.80

STN INTERNATIONAL LOGOFF AT 15:58:10 ON 08 JAN 2008